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# Large Eddy Simulation of Fire Phenomena

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## ABSTRACT

An approach to the simulation of gas phase fire phenomena based on the computation of the convection and combustion processes directly from the governing equations is presented. The methodology involves the explicit calculation of the large eddy structure induced by the fire from the geometric length scales describing the fire scenario down to a few centimeters. These computations are coupled to a local scale "thermal element" model which solves the equations governing combustion and radiation processes in a local coordinate system moving with the large scale motion. The basic theory behind the methodology is outlined and sample results of computations of both large and small scale phenomena are presented.

## 1. INTRODUCTION

There exists a variety of approaches to the simulation of fires in enclosures. One way of classifying them is according to the spatial and temporal resolving power of the method employed. Thus, zone models resolve transport processes in a multi–room building at the level of an individual room or passageway in the structure, with a minimum temporal resolution of order several seconds. Conventional field models using k–ε type representations of "turbulence" resolve such processes at the smaller geometric scales associated with individual rooms or portions of a room. The temporal resolution is effectively unchanged due to the need for some kind of averaging process inherent in such models. The approach outlined here, by contrast, seeks to solve the governing equations directly (if approximately) by considering transport and combustion phenomena in parallel, allowing each to evolve separately on their own length and time scales. These scales range from tens of meters to a fraction of a millimeter in length, and from tens of seconds to hundredths of a second in time.

The computational resources required by these approaches increase by several orders of magnitude as one spans the range of models and the complexity of the scenarios under consideration. Thus, progress in any of them is as strongly conditioned by advances in computer technology as it is in improved understanding of the underlying fire processes. This paper will attempt to demonstrate that there has been enough progress in both fields for large eddy simulations to be a viable tool in fire research. Indeed, the current status of large eddy simulations is very similar to that of k – ε field models about ten years ago. The remainder of the paper consists of a brief description of the theoretical basis for the present approach, followed by sections describing the large scale convective transport and the local scale "thermal element" model of combustion and radiation. Finally, a preliminary assessment of the prospects for this approach concludes the paper.

## 2. THEORY

Since the wide range of length and time scales to be considered is primarily due to the complex nature of the fire induced flow field, the starting point for the analysis is the fact that the velocity vector **u** can always be decomposed into a solenoidal field **v** plus an irrotational flow derived from a potential $\phi$. Under the usual conditions associated with low speed flow and combustion phenomena, these quantities can be related to the fluid vorticity $\omega$ and the thermal (combustion and radiative) volumetric sources or sinks of energy q as follows:

$$\nabla \times \mathbf{v} = \omega , \qquad \nabla \cdot \mathbf{v} = 0 . \tag{1}$$

$$\gamma/(\gamma - 1)\, P(t)\, \nabla^2 \phi + P'(t)/(\gamma - 1) = \nabla \cdot (k \nabla T) + q . \tag{2}$$

Here, $\rho$, P, k, and T are respectively the density, average enclosure pressure, thermal conductivity and temperature in the gas . Physically, the vorticity controls the large scale mixing of the smoke and hot gases, which is described by the solenoidal velocity component **v**. The potential $\phi$ is basically an expansion field driven by the net chemical heat release (allowing for radiative losses) q. This can be made even clearer by introducing a modified potential $\Phi$ defined as:

$$\phi = \Phi + ((\gamma - 1)/\gamma\, P(t)) \int k\, dT \quad , \qquad \gamma\, P(t)\, \nabla^2 \Phi = (\gamma - 1)\, q \; - P'(t) \tag{3}$$

In this form, the modified potential equation is a pure expansion field driven by combustion and radiation. Both $\Phi$ and **v** are primarily large scale fields, responsible for the motion of the smoke and hot gas transport throughout the building. The thermal source, however, is determined by small scale diffusive and radiative emission processes that act locally in the neighborhood of the gasified fuel. The major difficulty arises from the fact that the burning fuel is itself carried about by the large scale transport processes. The difficulty is resolved in the present approach by postulating that the gasified fuel can be represented by a large number of discrete elements. The elements are convected by the large scale motion and release heat at a rate to be determined. Since the combustion and emission processes are at too small a scale to be resolved as part of the large scale flow, they are represented for this purpose in the form:

$$q = \textstyle\sum_i q_i(t)\, \delta(\mathbf{r} - \mathbf{R}_i(t)) \quad , \quad \mathbf{R_i}'(t) = \mathbf{u}(\mathbf{R}_i(t), t) \quad . \tag{4}$$

Here, **r** and t are the general position and time coordinates, $\mathbf{R}_i(t)$ is the position of the $i^{th}$ fuel elment, $q_i(t)$ is the net heat release rate for that element, and $\delta$ denotes a delta function. The energy equation for the large scale motion is then:

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) - P'(t) = \nabla \cdot (k \nabla T) + q \quad . \tag{5}$$

Finally, the solenoidal velocity **v** is determined from the momentum equation which can be written as:

$$\frac{\partial \mathbf{v}}{\partial t} + \omega\times\mathbf{u} + \nabla\Pi/\rho_\infty - (1 - \rho/\rho_\infty)\mathbf{g} + (1 - \rho/\rho_\infty)\nabla p/\rho = \nabla\cdot(\mu\,\mathbf{def}(\mathbf{v} + \nabla\phi))/\rho \tag{6}$$

$$\Pi = p + \rho_\infty\left(\frac{\partial\phi}{\partial t} + \mathbf{u}^2/2\right) \;, \quad \mathbf{def}(\mathbf{u}) = \frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} - \frac{2}{3}\nabla\cdot\mathbf{u}\,\delta_{ij} \;. \tag{7}$$

The quantity p is the perturbation in pressure induced by the motion, **g** is the acceleration due to gravity, and $\mu$ is the viscosity of the gas. Note that the combination of equations (3) and (5) implies mass conservation [1] and that the first four terms on the left hand side of equation (6) are the dominant terms for a buoyancy driven flow at high Reynolds numbers. The net heat release $q_i(t)$ is determined by the thermal element model which will be discussed below.

## 3. LARGE SCALE TRANSPORT

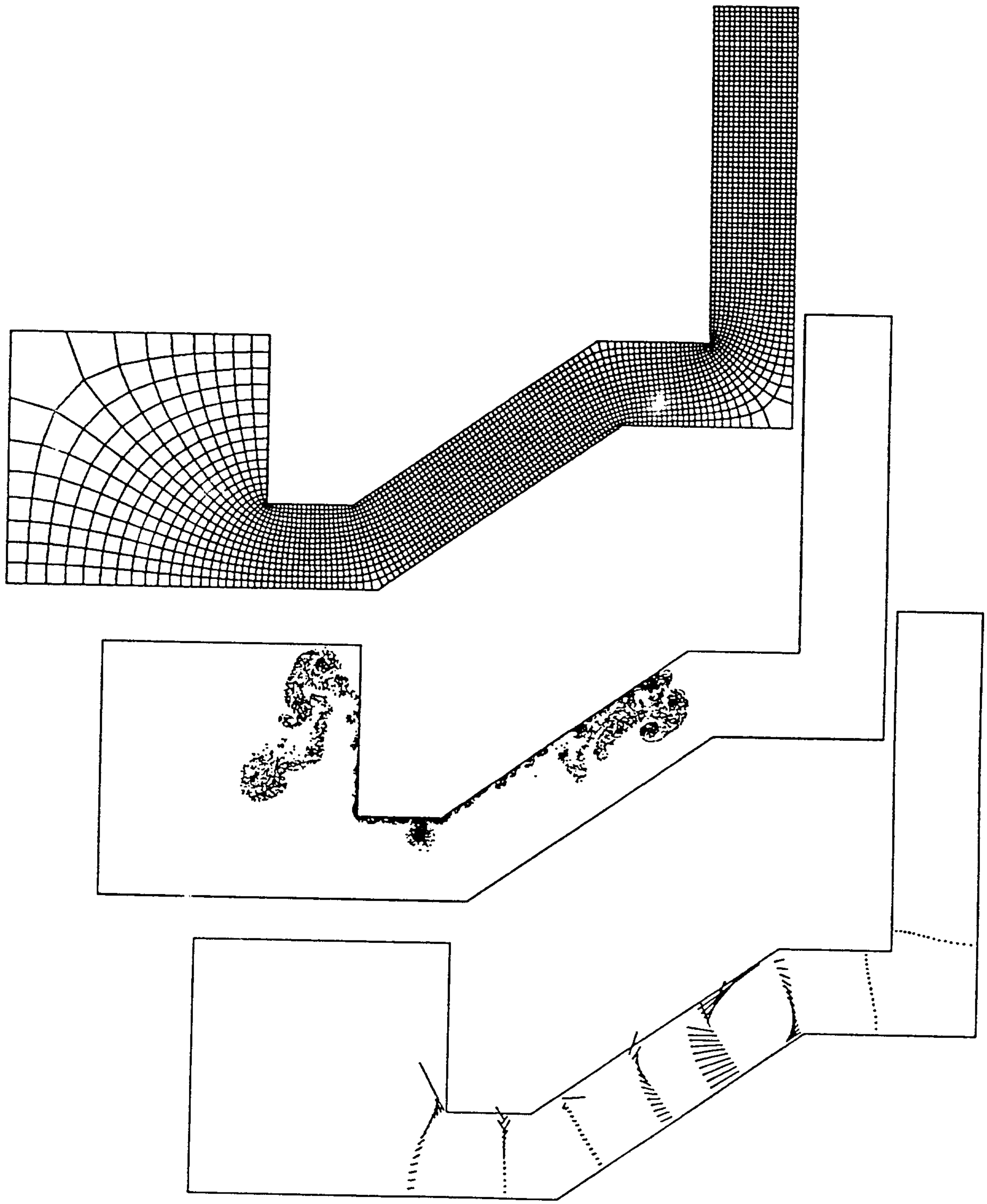
Calculations to date have concentrated on solving for the solenoidal velocity component **v** in two space dimensions. Away from the combustion zone this is the dominant contribution to large scale transport, and in this region the Boussinesq approximation is valid. Indeed, it is the basis for the salt/fresh water analogy for fire driven flows [2]. Mathematically, this amounts to retaining only the dominant terms on the left hand side of equation (6), replacing the density and transport properties by their reference values, and ignoring the contribution of the expansion potential $\phi$. Since the thermal element model outlined below is not yet connected to the large eddy simulation, $q_i(t)$ is taken as a prescribed function of time. Note that this still retains the essential feedback of a combustion model since the location of each burning element is determined by the large scale flow which is driven by the heat release.

Within these limits very detailed calculations have been performed for a variety of geometries [3]. The geometrical effects are accounted for by using a conformal transformation of the spatial coordinates to map a general polygonal domain into a rectangle. Figure 1 shows a plot of the "skeleton" of the conformally mapped grid used to calculate fire induced transport in the configuration shown. Each computational cell shown is actually subdivided into a 16 × 16 conformal grid. The full grid is 256 × 3072 uniforrmly spaced cells in a 1× 12 rectangle mapped into the space shown. The calculations are actually performed using dimensionless quantities defined with asterisks as follows:

$$\mathbf{r} = h\,\mathbf{x}^*, \quad t = (h/U)\,t^*, \quad p = \rho_\infty U^2 p^*, \quad \rho = \rho_\infty \rho^*, \quad T = T_\infty T^*, \quad \mathbf{u} = U\,\mathbf{u}^*,$$

$$U = (Q\,g/(\rho_\infty c_p T_\infty))^{1/3} \tag{8}$$

Here, h is the height or width of the narrow passages and Q is the average total heat release rate. The large area at the end of the horizontal passage has dimensions 3 h in both



Figures 1 –3. Skeleton of the computational grid used for large eddy simulation (top). Each cell shown is actually a conformal 16x16 grid. Locations of 10,000 thermal elements used to simulate the combustion at dimensionless time t* = 10 (center). The particles enter the enclosure near the ceiling of the lower horizontal corridor. Velocity vectors at selected stations in the skeleton grid at dimensionless time t* = 10 (bottom).

directions, and the overall horizontal and vertical dimensions of the enclosure are 9 h and 7 h respectively. Thus if h is three meters, the underlying computational grid has cells ranging in size from 1.2 cm. in the narrow passageways to a maximum of 7.2 cm. in the large room. Figure 2 shows the location of the burning (or burnt) thermal elements 10 dimensionless units of time (see eq.(8)) after flames started emerging from a region near the ceiling of the lower horizontal portion of the corridor. This scenario can be thought of as generated by burning gases entering through a transom above a door connecting a room adjacent to the corridor.

The range of dynamically active length and time scales is controlled by specifying a Reynolds number based on U and h. For the calculations shown here, the value 40,000 is used. Note that this corresponds to a global Reynolds number of order 300,000 based on the overall dimensions of the enclosure. The grid described above is sufficiently dense to support calculations that will resolve the three orders of magnitude range in dynamically active scales implied by this geometry and choice of parameters. This can be readily observed in the fine scale eddy structure displayed in Figure 2. Other quantities, such as velocity profiles at selected locations (Figure 3) can be readily determined.

## 4. THERMAL ELEMENT MODEL

The actual heat release process is determined on a local scale in a frame of reference moving with the large scale motion as calculated from the second of equations (4).Viewed in this way, the combustion process is described as the burning of and radiative emission from a spherically symmetric fuel element. This implies that the dominant local velocity is a combustion induced expansion, described in effect by equation (3). The combustion model assumes diffusion limited burning, and radiation from soot. In the absence of a generally used soot formation model, it is assumed that a specified fraction of the fuel is converted to soot immediately adjacent to the flame sheet on the fuel side.

The gaseous species are described in terms of a mixture fraction Z defined as:

$$Z = (\upsilon Y_f - Y_o + Y_\infty)/(\upsilon + Y_\infty) \tag{9}$$

Here, $\upsilon$ denotes the stoichiometric mass of oxidizer required per unit mass of fuel, while $Y_f$ and $Y_o$ are the fuel and oxidizer mass fractions respectively. The species conservation equations can then be written in terms of a radial expansion velocity u and diffusivity D as:

$$\rho r^2 \left(\frac{\partial Z}{\partial t} + u \frac{\partial Z}{\partial r}\right) = \frac{\partial}{\partial r}\left(\rho D r^2 \frac{\partial Z}{\partial r}\right) \tag{10}$$

The optically thin energy equation for a gas with an emissivity $\kappa$ per unit mass of soot is:

$$\rho r^2 \left(\frac{\partial H}{\partial t} + u \frac{\partial H}{\partial r}\right) = \frac{\partial}{\partial r}\left(\rho D r^2 \frac{\partial H}{\partial r}\right) - \rho_s r^2 \kappa \theta (T^4 - T_\infty^4)/(c_p T_p - c_p T_\infty + q_o) \tag{11}$$

The quantity H is a thermal Zeldovich variable defined by:

$$H = (c_pT + q_oY_f - c_pT_\infty)/(c_pT_p + q_o - c_pT_\infty) \tag{12}$$

The quantity $q_o$ is the heat released per unit mass of fuel burnt, $T_p$ is the unburnt fuel pyrolysis temperature, $\rho_s$ is the soot solid density, and $\theta$ is the soot volume fraction. The soot mass evolution equation is assumed to be:

$$\rho_s\left(\frac{\partial\theta}{\partial t} r^2 + \frac{\partial}{\partial r}((u + u_t)\, r^2\, \theta)\right) = \beta\, r^2\, m_f \tag{13}$$

The thermophoretic velocity $u_t$ is related to the temperature gradient as follows [4]:

$$u_t = -\,0.55\,(\mu/(\rho\, T))\,\frac{\partial T}{\partial r} \tag{14}$$

Note that the radial velocity u is determined from solving equation (3) in local spherical coordinates. The solution ensures that mass is conserved in each thermal element. This fact together with the large scale formulation guarantees that mass is conserved everywhere. Thus, the thermal element model is a solution of the mass, energy, and species conservation equations on both small and large scales.

The fuel mass consumption rate per unit volume $m_f$ is determined from the flux of fuel into the flame sheet while the fraction of the fuel burned converted to soot $\beta$ is at present an empirically determined quantity. However, the fraction of the energy release converted into thermal radiation is calculated directly from the model. The only additional assumption required is that absorption of radiation into each thermal element can be ignored. Since the net energy release rate $q_i(t)$ for any fuel element is equal to the thermal energy released over the flame sheet surface minus the fraction radiated away, the solution to the above equations yields all of the information required for the large eddy simulation.

Figure 4 shows the time history of the chemical energy released and the amount radiated away for a 1 centimeter propane element initially at ambient temperature. The results are presented in terms of an expansion rate since that is how they enter the calculation of the large scale velocity field. The early time high expansion rate is a consequence of the diffusion away from a discontinuous initial state. The absolute level of the radiation is low since it is assumed that only 2 percent of the fuel burnt is converted to soot. The radiant energy loss first increases as soot is generated and the flame expands, and then decreases as the soot shell cools. Note that even after combustion ceases due to fuel burnout, thermal energy is still lost by radiation. The fraction of the total energy released up to time t that is radiated away is shown in figure 5. Even though the rate of loss is relatively small, the integrated effect is large enough so that at burnout 38 percent of the chemical energy released has been radiated away. The model contains a variety of interesting combustion phenomena, which will be described in detail elsewhere [5]. A sample of the detail contained in the model is shown in figure 6, which displays a contour plot of the temperature field in the burning

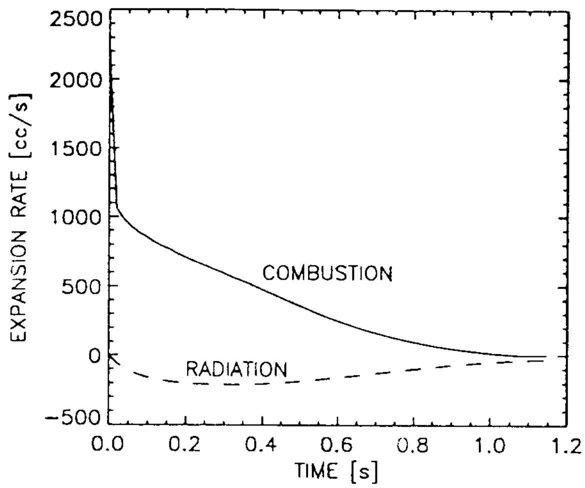



Figure 4. Time history of chemical energy release rate and radiative emission for a 1 cm. propane element.

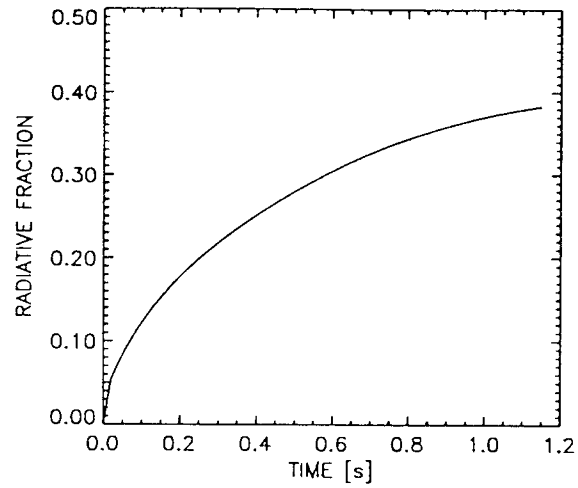



Figure 5. Cumulative fraction of chemical energy lost through radiation.

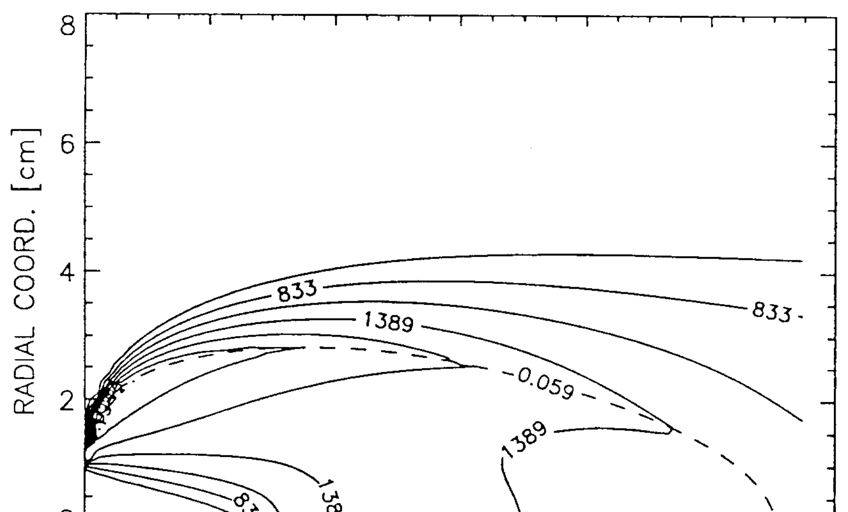



Figure 6. Contour plot of temperature in propane fuel element. The numbers on the solid lines are temperatures in Kelvin. The dashed line is the flame sheet location with the value of the mixture fraction on the sheet indicated.

propane element. Note the initial outward movement of the flame sheet as it seeks the oxygen, followed by a subsequent collapse as the fuel is consumed.

## 5. FUTURE PROSPECTS

The utility of the approach described above depends on the resolution of two issues: the coupling of the large scale transport and small scale combustion calculations, and the extension of the large scale transport to three space dimensions. At the time of writing, the work needed to accomplish the first task is under way and should be completed for the two dimensional case within a year. The second issue, three dimensional large scale transport, is largely one of computer resources. The calculations reported above were all performed on an IBM RS/6000 model 550 compute server, which costs well under US$ 100,000. The computations took tens of hours to complete for the example shown. A three dimensional calculation for a room of the size used in the famous bedroom fire experiments performed under the direction of Prof. H. Emmons would require comparable time on a Cray Y/MP supercomputer. (These computers are singled out because the author and his collaborators have access to them. Other manufacturers produce comparable machines). However, the performance of compute servers and other microprocessor based computers is rapidly increasing. In fact, computations on small machines at the levels of performance required to carry out such computations will be available in 2 to 3 years. This takes no account of any possible breakthroughs in parallel computing. Indeed, it would be surprising if three dimensional calculations at resolutions within a factor of two of that shown above in small buildings were not possible by the end of the decade. Since these calculations are directly based on the laws of physics, they should provide a rich understanding of the mechanisms of combustion and transport in fires.

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